Pimelic acid, 4-chloro-3-methylphenyl octyl ester

Inchi: InChI=1S/C22H33ClO4/c1-3-4-5-6-7-11-16-26-21(24)12-9-8-10-13-22(25)27-19-14-15-20

InchiKey: GWWKDXQAMJOJJH-UHFFFAOYSA-N

Formula: C22H33ClO4

SMILES: CCCCCCCCOC(=O)CCCCCC(=O)Oc1ccc(Cl)c(C)c1

Mol. weight [g/mol]: 396.95

Physical Properties

Property code	Value	Unit	Source
gf	-252.26	kJ/mol	Joback Method
hf	-789.16	kJ/mol	Joback Method
hfus	55.77	kJ/mol	Joback Method
hvap	90.86	kJ/mol	Joback Method
log10ws	-7.25		Crippen Method
logp	6.408		Crippen Method
mcvol	324.200	ml/mol	McGowan Method
pc	1130.62	kPa	Joback Method
rinpol	2969.00		NIST Webbook
rinpol	2969.00		NIST Webbook
tb	929.41	K	Joback Method
tc	1140.08	K	Joback Method
tf	563.40	K	Joback Method
vc	1.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1023.57	J/mol×K	929.41	Joback Method
cpg	1038.87	J/mol×K	964.52	Joback Method
cpg	1052.89	J/mol×K	999.63	Joback Method
cpg	1065.66	J/mol×K	1034.75	Joback Method
cpg	1077.20	J/mol×K	1069.86	Joback Method
cpg	1087.55	J/mol×K	1104.97	Joback Method
cpg	1096.72	J/mol×K	1140.08	Joback Method
dvisc	0.0003410	Pa×s	563.40	Joback Method

dvisc	0.0001951	Pa×s	624.40	Joback Method
dvisc	0.0001233	Pa×s	685.40	Joback Method
dvisc	0.0000840	Pa×s	746.41	Joback Method
dvisc	0.0000606	Pa×s	807.41	Joback Method
dvisc	0.0000458	Pa×s	868.41	Joback Method
dvisc	0.0000359	Pa×s	929.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416688&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume